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TITLE: THE EVALUATION AND APPLICATION OF REDUNDANT-CROSS-SECTION COVARIANCES

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THE EVALUATION AND APPLICATION OF REDUNDANT-CROSS-SECTION COVARIANCES

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ABSTRACT

Certain multigroup covariance libraries, notably COVFILS-2, omit all redundant (or summed) reactions on the grounds that the information content of a well-measured total cross section, for example, is implicitly contained in the covariances of the component, or partial, reactions that add up to the total. We analyze this strategy and show that, while redundant reactions can play an important role in cross-section and covariance evaluation, their emission from libraries intended for applications is justifiable.

We consider the problem of estimating the uncertainty in some function f(u), induced by the uncertainties in the cross-section set u. Normally, some of the reactions affecting f are "redundant" having cross sections that are, by definition, obtainable by simply summing the cross sections for particular non-redundant (NR) reactions. Examples of typical redundant reactions are the total, nonelastic, and total inelastic reactions. Certain multigroup covariance libraries, notably COVILS-2,[1] omit all redundant reactions on the grounds that the information content of a well-measured total cross section, for example, is implicitly contained in the covariances of the component, or partial, reactions that add up to the total. In this paper, we analyze this strategy in some detail. While redundant reactions can play an important role in cross-section evaluation, we conclude that their emission from libraries intended for sensitivity and uncertainty analysis can be justified, provided the cross-section and covariance data have been evaluated consistently.

Suppose that the function f(u) is at least approximately linear in the neighborhood of some reference point $\{u_{i,ref}\}$, where it takes on the value

$$f_{ref} = f[u_{i,ref}] \tag{1}$$

In the neighborhood of the reference point, we can, to a good approximation, write

$$f = f_{ref} + \sum_k c_k [u_k - u_{k,ref}] \quad , \tag{2}$$

where the index k runs over all reaction types and over all energies. We can simplify Eq. (2) by collecting all of the constant terms together,

$$f_0 = f_{ref} - \sum_k c_k u_{k,ref} \quad , \tag{3}$$

so that

$$f - f_0 = \sum_k c_k u_k \quad . \tag{4}$$

We next rewrite Eq. (4) with a slight notational change, in order to emphasize the separate contributions of the two types of data,

$$f - f_0 = \sum_i a_i s_i + \sum_j b_j t_j \quad , \tag{5}$$

where i ranges over all non-redundant reaction types (with cross sections s_i) and over all energies, and j ranges over all redundant reaction types (with cross sections t_j) and over all energies.

We next introduce row vectors A and B, containing the a_i and b_j, respectively, and the column vectors S and T, containing the s_i and t_j. Then Eq. (5) becomes

$$f - f_0 = A\,S + B\,T \quad . \tag{6}$$

The fixed relationship of the two types of data can be written as

$$T = H\,S, \tag{7}$$

where H is a rectangular matrix of constant coefficients, normally having magnitude zero or unity. Combining Eqs. (6) and (7) gives us an alternate form for f,

$$f - f_0 = K\,S \quad , \tag{8}$$

where

$$K = A + B\,H \quad .$$

We now turn to the subject of covariances. It is useful, at least conceptually, to break the evaluation process into two parts. We suppose that the

vector S is initially determined by use of direct measurements, and these measurements have a covariance, or dispersion, matrix D(S). We assume that T is initially determined strictly by "theory," T = H S. At this point then, all covariances are determined entirely by the measurement uncertainties of S.

In the second step, one incorporates direct measurements M of the redundant cross sections into the covariance assessment. The M play a role exactly analogous to the integral measurements in a conventional, neutronics-oriented statistical "adjustment" exercise, while the S play the role of the differential data. Because of this clear equivalence, we shall use the term "adjusted" to refer to the data evaluator's final combined evaluation of the redundant and NR cross sections. The final, or adjusted, values will be identified in our discussions by the use of the prime symbol (').

The new information provided by the measurements M is most compactly expressed in terms of the "discrepancy" vector P,

$$P = M - T = M - H S \quad . \tag{10}$$

In Ref. 2, it is shown under very general conditions that, given P and its pre-adjustment covariances D(P), the "best" (minimum-variance) estimate for an arbitrary vector Z is given by

$$Z' = Z - \mathrm{cov}(Z,P)\ G\ P \quad , \tag{11}$$

with covariances

$$D(Z') = D(Z) - \mathrm{cov}(Z,P)\ G\ \mathrm{cov}(Z,P)^{\dagger} \quad , \tag{12}$$

where

$$G = [D(P)]^{-1} \quad . \tag{13}$$

In these relations, the elements of the vector Z can be any quantity that "covaries" with P: differential data, functions of the data (even nonlinear functions), or a mixture of data and functions. The notation cov(Z,P) denotes a rectangular matrix whose ij-th element is the pre-adjustment covariance $\mathrm{cov}(z_i, p_j)$, and the symbol (†) denotes the matrix transpose.

Equations (11)-(13) can be applied immediately to the problem of combining the redundant and NR measurements. First, we identify the arbitrary matrix Z with the redundant cross sections T. The adjusted values are then given by

$$T' = T - \mathrm{cov}(T,P)\ G\ P \quad . \tag{14}$$

The adjusted NR values are similarly obtained by identifying Z with S,

$$S' = S - \mathrm{cov}(S,P)\ G\ P \quad . \tag{15}$$

Covariances, such as D(T') and D(S') are immediately obtainable from Eq. (12) with these same identifications.

Equations (14) and (15) provide the optimum evaluated results for all cross sections, taking full account of all available measurements. Of course, stating that this approach is optimum does not mean that all evaluations in a file such as ENDF/B were performed in this way. Even so, this indicates the desired direction that evaluations should take, in order to extract the maximum possible information content from available experimental data.

In fact, a large number of current evaluations do follow this path, at least to the extent of using well-measured total cross sections as a constraint in determining the less well-known reactions, such as elastic scattering. In the covariance files, the frequently occurring statement that reaction-type 2 (MT2) is "derived" in some energy range, from the relation MT1 - MT102, for example, directs the multigroup processing program to reconstruct[3] all covariances involving MT2 in that energy range. In the usual use of this format (an "NC-type" sub-subsection with LTY = 0), the evaluator is, in effect, making the approximation that the covariances of the direct measurements of MT2 are essentially infinite. The experimental data and the associated covariances for MT1 and MT102 would be completely unchanged by an adjustment, Eqs. (11)-(15) in this case (because G approaches 0), so they can go directly into the data file as "measured." The "derived" covariances calculated for MT2 by the processing program are identical to what the evaluator would have obtained, using Eqs. (11)-(15) with very large input covariances for MT2.

It is still mathematically correct to use the LTY = 0 format when the covariances for MT1 and MT102 (to continue with our example) have been substantially adjusted, and this is sometimes done, even though this was not the intent

of the original proposers of this format. In such cases, the adjusted covariances for MT1 and MT102 are placed in the file, and adjusted covariances for MT2, although known to the evaluator, are again left to be reconstructed by the processing program. In this case, the use of the LTY = 0 format is not a transparent statement about the method of evaluation, but merely a mechanical convenience to shorten the data files. (The number of reaction pairs is reduced from six down to three in our example.) The use of LTY = 0 is still possible here because the mathematical connection between the final covariances for the three reactions is the same, whatever magnitude is assumed for the covariances of the direct measurements of MT2.

Evaluations that do not follow the approach, described in the preceding paragraphs, of enforced consistency between the data and covariances for various reactions (incorporating, for example only direct-measurement covariances for MT1, MT2, and MT102 and ignoring the logical connection) are seriously flawed and are thus clear candidates for re-evaluation. On this bases, we assume that the evaluations of the more important materials either are already "consistent," in the above sense, or soon will be. This is important, because, when creating processed covariance libraries from consistent evaluations, one can dispense with redundant reactions entirely. To show this. we calculate the uncertainty in the post-adjustment value of f.

$$\mathrm{var}(f') = \mathrm{var}(f' - f_0) = \mathrm{var}(A\,S' + B\,T')$$

$$= \mathrm{cov}(A\,S' + B\,T',\ A\,S' + B\,T')$$

$$= A\,D(S')A^{\dagger} + A\,\mathrm{cov}(S',T')B^{\dagger} + B\,\mathrm{cov}(T',S')A^{\dagger} + B\,D(T')\,B^{\dagger} \quad . \quad (16)$$

ENDF/B-V provides, in general, covariance information for both redundant and NR data. Covariance processing programs, such as the ERRORR module[3] of NJOY, can easily retrieve all of the covariances and put them out in the multigroup structure specified by the code user. The question at hand is whether all, or just a portion, of these output covariances actually need to be incorporated into multigroup covariance libraries in order to permit the computation of uncertainties such as var(f'). Superficially, it would seem that all are required, because three of the four terms in Eq. (16) involve the uncertainties of T'. This first impression turns out to be untrue. To show why, we first multiply Eq. (15) from the left by H, yielding

$$H\,S' = H\,S \quad H\,\mathrm{cov}(S,P)\,G\,P = T - \mathrm{cov}(T,P)\,G\,P \quad , \tag{17}$$

where the last result follows from Eq. (7). Comparing Eqs. (17) with Eq. (14), we see that

$$T' = H\,S' \quad . \tag{18}$$

Putting Eq. (18) into words, the best estimates of the functions are equal to the functions of the best estimates of the data. Because of the existence of this simple linear connection (even after taking into account direct measurements of both types of reaction and correlations between the two), the uncertainty in the redundant data can still be propagated from the uncertainty of NR data. We can use this fact to simplify Eq. (16),

$$\mathrm{var}(f') = A\,D(S')A^{\dagger} + A\,\mathrm{cov}(S',\,H\,S')B^{\dagger} + B\,\mathrm{cov}(H\,S',\,S')A^{\dagger} + B\,\mathrm{cov}(H\,S',H\,S')B^{\dagger}$$

$$= A\,D(S')\,(A^{\dagger} + H^{\dagger}\,B^{\dagger}) + B\,H\,D(S')\,(A^{\dagger} + H^{\dagger}\,B^{\dagger})$$

$$= (A + B\,H)\,D(S')\,(A + B\,H)^{\dagger} \quad .$$

Recalling Eq. (9), we have simply

$$\mathrm{var}(f') = K\,D(S')\,K^{\dagger} \quad . \tag{19}$$

Equation (19) summarizes our main conclusion, namely, that sensitivity and uncertainty analysis does <u>not</u> require covariances of the redundant cross sections.

In addition to saving space in a covariance library such as COVFILS-2, there is an additional reason for restricting the library to the subset of non-redundant reactions. Sensitivity-analysis programs are specifically coded to calculate the effect on f, for example, of changing a single NR cross section while holding all other NR reactions fixed. In this process, redundant cross sections are allowed to change in response to changes in their NR components. This is exactly the point of view adopted in deriving Eq. (8). The calculated sensitivities can thus be immediately identified with the elements k_i of the vector K. With the k_i in hand, one is immediately ready to calculate the uncertainty in f using Eq. (19). The vectors A and B, on the other hand, are fundamentally ambiguous.

To illustrate this point, consider a case in which there is a single redundant reaction, namely the total so that $t = u_{tot}$ for some specified energy group. One can simply define the coefficient b to be, for example, the rate of change of f with respect to a correlated change in all partial reactions in that group, holding all partial-to-partial ratios constant. Other definitions are also possible. Since there is only one redundant reaction, the matrix H is just a row vector, and it contains all ones. The matrix product B H is also a row vector, with an entry of b in each position. Once b is specified, the elements of A are then determined by Eq. (9),

$$a_i = k_i - b \quad . \tag{20}$$

Thus, one can, indeed, include redundant reactions explicitly in a sensitivity and uncertainty analysis, but only if one simultaneously reduces the NR-reaction sensitivities so as to cancel the net effect of this inclusion. There seems to be little point to performing the analysis in this way.

REFERENCES

1. D. W. Muir, "COVFILS-2: Neutron Data and Covariances for Sensitivity Analysis," Fusion Tech. 10 (3), part 2B (November 1986).

2. D. W. Muir, "The Use of Perturbed Libraries in the Design and Analysis of Integral Experiments," in E. D. Arthur and A. D. Mutschlecner, Comps., Applied Nuclear Science Research and Development Semiannual Progress Report: December 1, 1985-June 30, 1986," Los Alamos National Laboratory report (to be published), pp. 63-67.

3. D. W. Muir and R. E. MacFarlane, "The NJOY Nuclear Data Processing System, Volume IV: The ERRORR and COVR Modules," Los Alamos National Laboratory report LA-MS-9303, Volume IV (January 1986).